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# Supplementary Information

# CFD-accelerated bioreactor optimization: Reducing the hydrodynamic parameter space

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## 1 Calculation of total power requirement

In the design of the AFBR, there are many sources of pressure loss such as pipe fittings, the particles, diffusers and other frictional losses. In this appendix, we consider three major sources of pressure loss, namely fluidization, hydrostatic pressure due to elevation and friction loss due to the pipes. The total power requirement $P_{loss}$ is defined as

$$P_{loss} = \rho_f g \Big( h_{GAC} + f \frac{L}{D_{pipe}} \frac{u_{pipe}^2}{2g} + h_{static} \Big), \tag{1}$$

where $h_{GAC}$ is the head loss due to fluidization of the GAC particles, $D_{pipe}$ is the length of the recirculation pipe, $u_{pipe}$ is the flow speed in the recirculation pipe, $\rho_f$ is the density of water, $g$ is the gravitational acceleration, $h_{static} = H_f$ is the elevation difference and $f$ is the friction factor.

To calculate $h_{GAC}$, we apply Ergun's relationship

$$u_{mf} = \frac{g d_p^2 (\rho_p/\rho_f - 1)}{150 \nu_f} \frac{(1-\phi_{mf})^3}{\phi_{mf}}, \tag{2}$$

where $\phi_{mf} = 0.52$ is the volume fraction of close-packed particles and

$$h_{GAC} = \frac{150 \nu_f H_0}{g d_p^2} \frac{\phi_{mf}^2}{(1-\phi_{mf})^3} u_{mf} + \frac{1.75 H_0}{g d_p} \frac{\phi_{mf}}{(1-\phi_{mf})^3} u_{mf}^2, \tag{3}$$

where $H_0 = H_f \phi / \phi_{mf}$ is the height of a close-packed bed and $\phi$ is the volume fraction of the fluidized bed given an upflow velocity $u_0$. The volume fraction can be estimated with the power law relationship

$$\phi = 1 - \Big( \frac{u_0}{k w_t} \Big)^{1/n}, \tag{4}$$

where $k$ is a constant in the range $0.7 - 0.9$, $w_t$ is the settling velocity of a single particle in the domain of interest and $n$ is the expansion index that can be estimated from the relationship

$$n = \frac{5.1 + 0.27 Re_t^{0.9}}{1 + 0.1 Re_t^{0.9}}, \tag{5}$$

where $Re_t = w_t d_p/\nu_f$ is the terminal Reynolds number. The friction factor can be calculated with the modified Colebrook White equation

$$f = \frac{0.25}{\log\left(\frac{\zeta}{3.7D_{pipe}} + \frac{5.74}{Re_{pipe}^{0.9}}\right)}, \tag{6}$$

where $\zeta = 0.0015$ is the typical roughness coefficient of a PVC pipe and $Re_{pipe} = u_{pipe}D_{pipe}/\nu_f$ is the pipe Reynolds number based on $u_{pipe} = 4Q_r/(\pi D_{pipe}^2)$, where $Q_r = u_0 A$ is the recirculation flow rate and $A$ is the cross sectional area of the recirculation flow pipeline. We assume the reactor dimensions such that $L = 4.3$ m, $H_f = 2$ m and $A = 1.4$ m$^2$. Different $Ar$ are achieved by using a particle diameter of $d_p = 2$ mm and particle densities of $\rho_p = 1300$, 2600 and 4000 kg m$^{-3}$.